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Simulation of X-ray diffraction-line broadening for a material containing misfitting precipitates

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Abstract

The locally varying strain field in a matrix containing misfitting second phase particles and its effects on diffraction-line broadening have been simulated numerically. A two-dimensional model material has been considered: A matrix with a periodic arrangement of misfitting circular second phase particles. The strain field is calculated numerically from a micro mechanical model that in principle takes into account the elastic interaction of the misfitting particles. Diffraction-line profiles have been calculated as a function of particle fraction and particle/matrix misfit. Shifts and broadenings of these line profiles have been discussed with reference to known characteristics of Eshelby's approach for point imperfections. © 1997 Elsevier Science S.A.

Keywords: X-ray diffraction-line broadening; Micromechanical modelling; Misfitting particles

1. Introduction

The mechanical properties of crystalline materials containing a dispersion of particles (precipitates, inclusions) can be controlled largely through the size and distribution of the second phase particles and the particle/matrix misfit. For instance, dislocation movement through such materials is dependent on the strain field surrounding the second phase particles due to the (volume) misfit of particle and matrix [1]. Hence, there is a strong need to characterize the strain field in matrix-particles assemblies in order to predict and control the mechanical properties.

Diffraction-line broadening is representative for the (distribution of) local strains. However, the interpretation of this diffraction-line broadening in terms of local strain fields is not straightforward [2]. Diffraction-line broadening can be conceived usually as caused by local variations in the lattice spacing (strain broadening) and the finite size of the diffracting crystals (size broadening)¹. Until now, methods used for line-profile decom-

position (i.e. size-strain separation) rely on specific assumptions made for the order dependences of the size and strain broadenings, leading to size and strain parameters that are difficult to interpret [2,3]. Recently, a different approach has been proposed: Line-profile simulation on the basis of an appropriate strain-field model. Treatments by Van Mourik et al. [4] and Van Berkum et al. [5] for the effect of misfitting particles on line broadening were based on a description of the particle induced misfit-strain field in the matrix according to a formulation by Eshelby for misfitting point defects [6]. Thus, the influence of the particle/matrix misfit and the volume fraction occupied by the particles on the simulated line profiles could be modelled readily. However, the interaction of the strain fields caused by the individual particles could not be accounted for, implying that these models pertain to cases of low particle volume fraction.

This study is devoted to the simulation of diffraction-line broadening for a simple two-dimensional model material containing a periodic distribution of circular misfitting particles. The calculation of the strain fields is based on a micromechanical model incorporating the effect of elastic interaction of misfitting particles. These first results deal with the effects of particle volume fraction and particle/matrix misfit on the centroids and

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¹ The so-called instrumental line broadening due to instrumental imperfections is not considered in this paper.

the broadenings of the diffraction-line profiles of the matrix for cases without elastic interaction.

2. Calculation of the strain field

Consider an infinitely large two-dimensional model sample of a material containing a square doubly-periodic array of identical circular particles. Due to this periodicity, the material can be represented by a square unit cell (size: $2L \times 2L$), containing a single, centered, circular particle (radius R), that is called the particle-arrangement unit cell. The atomic arrangement of the matrix (square array of $2N \times 2N$ atoms per particle-arrangement unit cell) is described by a square matrix unit cell (size: $L/N \times L/N$) containing a single, centered atom.

In this paper, both matrix and particle are assumed to be isotropic and purely elastic. The misfit between particle and matrix is characterised by the linear misfit parameter ϵ ². The displacement field and the strain field in the particle-arrangement unit cell are calculated using a finite element method on the basis of plain strain elasticity, applying periodic boundary conditions at the sides of the particle-arrangement unit cell such that the material is macroscopically stress-free. A four noded element [7] is applied that is reduced in size close to the particle-matrix interface due to the high strain gradients there.

The (hk) diffraction-line profile contains information on strain components in the $[hk]$ direction only. Therefore, from the computed strain-tensor field, the average local strain, $\langle e_{[hk]} \rangle$, and the root mean squared local strain, $\sqrt{\langle e_{[hk]}^2 \rangle}$, both in the $\{hk\}$ direction, have been calculated. These mean strain values scale linearly with the matrix/particle misfit ϵ .

3. Calculation of the line profile

3.1. Intensity distribution of a single powder particle

According to the kinematical theory of diffraction the (hk) intensity distribution of a single (here two-dimensional) crystal in reciprocal space is given by the square of the modulus of the product of the structure factor F and the crystal factor G [3,8]. The structure factor F for the $\{hk\}$ reflection is given by $F = \sum_n f_n e^{2\pi i(\mathbf{H} \cdot \mathbf{r}_n)}$ with f_n the atomic scattering factor of atom n at position \mathbf{r}_n in the unit cell considered and

$\mathbf{H} = h\mathbf{b}_1 + k\mathbf{b}_2$ is the so-called diffraction vector, where \mathbf{b}_1 and \mathbf{b}_2 denote the axes of the unit cell of the corresponding reciprocal lattice. The crystal factor G for the (hk) reflection can be written as $G = \sum_{m_1} \sum_{m_2} e^{2\pi i(\mathbf{H} \cdot \mathbf{R}_{m_1 m_2})}$ with $\mathbf{R}_{m_1 m_2} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2$ as the vector indicating the position of the (m_1, m_2) unit cell with \mathbf{a}_1 and \mathbf{a}_2 as the crystal axes pertaining to the unit cell considered. If all unit cells are exactly equal and the powder particle is 'infinitely large', it follows that G has only non-zero values for integer values of h and k . Hence, each (hk) line profile is a line intensity.

Now, describe the single powder particle as an assembly of particle-arrangement unit cells. These unit cells are all equally strained (although the matrix unit cells making up a particle-arrangement unit cell are differently strained) and therefore the intensity distribution in reciprocal space of the single powder particle consists of a series of line intensities. The same result would have been obtained if the single powder particle considered had been described in terms of an assembly of matrix unit cells. This implies that the $(h_{pa}k_{pa})$ reflection in terms of the particle-arrangement unit cell description corresponds with the (h_mk_m) reflection in terms of the matrix unit cell description. Although the matrix unit cells are strained differently, the (h_mk_m) line intensity observed for the unstrained condition, does not 'broaden' in the usual sense for the strained condition: Instead, this 'broadened' (h_mk_m) line profile is made up by a series of $(h_{pa}k_{pa})$ line intensities around the position of the ideal (h_mk_m) line intensity due to the periodicity of the second phase particle distribution. Therefore, in this work $(h_{pa}k_{pa})$ line intensities have been calculated for $h_m - (1/2) \leq h_{pa} \leq h_m + (1/2)$ and $k_m - (1/2) \leq k_{pa} \leq k_m + (1/2)$ to obtain the intensity distribution belonging to an (h_mk_m) -reflection in reciprocal space.

3.2. Intensity distribution of a powder specimen

Consider a powder composed of 'infinitely large' powder particles, each of which is identical to the powder particle considered above. The orientation distribution of the powder particles is perfectly random. Then, the intensity of the $\{h_mk_m\}$ powder diffraction-line profile at a specified length of the diffraction vector, $|\mathbf{H}|$, can be obtained from the intensity distribution in reciprocal space for a single powder particle as considered above, through an integration over the circumference of the circle with radius equal to $|\mathbf{H}|$ (cf. the case of 3D crystals: [8]). The full $\{h_mk_m\}$ powder diffraction-line profile is obtained by repeating this procedure for an appropriate range of diffraction vector lengths.

The $\{h_mk_m\}$ powder diffraction-line profiles thus generated, consisting of a series of line intensities, are

² For example, in the case of a thermal misfit the linear misfit ϵ equals $\Delta\alpha\Delta T$, with $\Delta\alpha$ the difference in thermal expansion coefficients of particle and matrix and ΔT the change in temperature.

characterized by their centroid \tilde{H} and their standard deviation S .

4. Results of parameter study and discussion

The present parameter study focusses on the effects of the particle/matrix linear misfit strain ϵ and the particle fraction c (the two-dimensional analogue of the volume fraction: $c = \pi R^2/4L^2$) on the centroid and the standard deviation of the simulated matrix line-profiles (in the intensity calculations $f_{\text{matrix atom}} = 1$ and $f_{\text{particle atom}} = 0$). In the calculations presented here $2N = 120$, thus representing a total of 14 400 atoms per particle-arrangement unit cell. The Young's moduli and Poisson ratios of matrix and particle in this first study have been taken equal: $E_m = E_p^3$, $\nu_m = \nu_p = 0.3$; this implies that in this study elastic interaction of the misfitting particles is not considered. The particle/matrix linear misfit strain ϵ is varied between 0 and 5% and the particle fraction is varied between $c = 0.35\%$ ($R = (1/15)L$) and $c = 19.6\%$ ($R = (1/2)L$). Attention is confined to the simulation of $\{h_m = h_{pa}/120 = 1, k_m = k_{pa}/120 = 1\}$ diffraction-line profiles.

Three simulated $\{11\}$ -matrix powder diffraction-line profiles are shown in Fig. 1 ($c = 8.7\%$, $\epsilon = 0, 2, 5\%$). The distribution of line intensities making up the line profile (cf. Section 3) shifts and broadens with increasing ϵ , as compared to the undeformed state ($\epsilon = 0$).

The line-profile shift, as exhibited by its centroid \tilde{H} , depends on the particle fraction c and the particle/matrix misfit ϵ , as illustrated in Fig. 2: Increases of ϵ

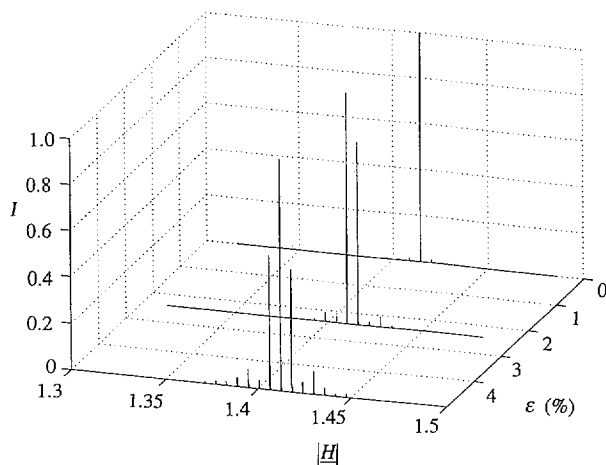


Fig. 1. Simulated $\{11\}$ intensity distribution with normalised intensity I (each intensity distribution is normalised through division by its maximum intensity) vs. length of diffraction vector, $|H|$, for $\epsilon = 0.0, 2.4$ and 5.0% .

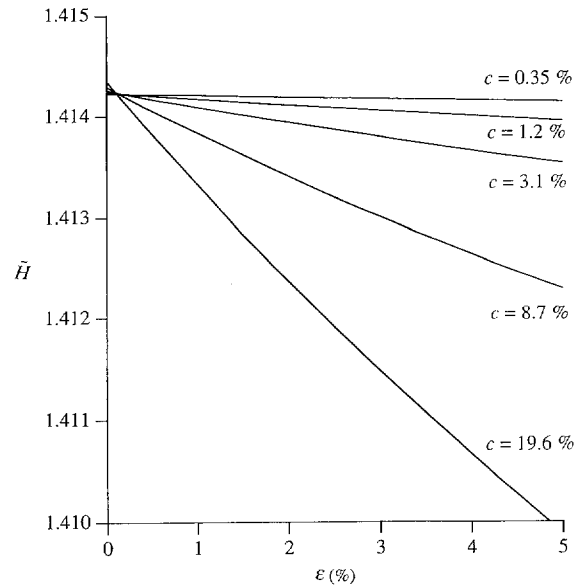


Fig. 2. Centroids \tilde{H} of the distribution of positions of the group of line intensities of the simulated $\{11\}$ -reflection vs. ϵ for various particle fractions c .

and/or c result in a shift of the centroid to smaller lengths of the diffraction vector, indicating an increase of the average distance between reflecting $\{11\}$ -planes. This is compatible with the calculated strain data: Positive values of $\langle e_{[11]} \rangle$ occur for the ϵ - and c -ranges considered (see Fig. 3). The micromechanical calculations also reveal a linear relation between $\langle e_{[11]} \rangle$ and the particle fraction c (Fig. 3); this agrees with results obtained using Eshelby's approach (e.g. eq. 1 in [5]), which is compatible with the absence of elastic interac-

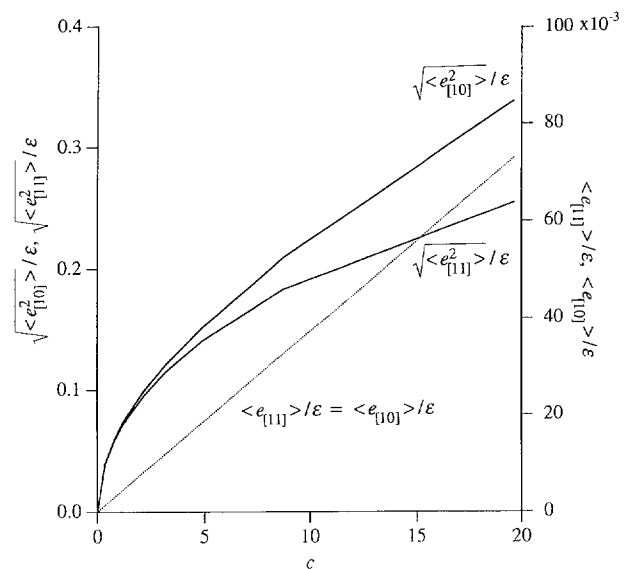


Fig. 3. Normalised mean strain and normalised root mean squared strain in the $[11]$ and $[10]$ direction (normalised through division with misfit strain ϵ) vs. c .

³ The actual values of $E_m = E_p$ is inconsequential for the strain field in the case considered here.

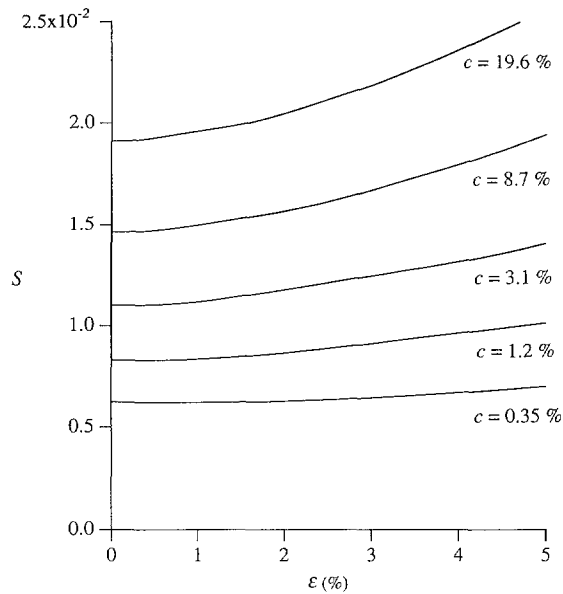


Fig. 4. Standard deviations S of the distribution of positions of the group of line intensities of the simulated $\{11\}$ -reflection vs. ϵ for various particle fractions c .

tion effects (the mechanical properties of precipitate and matrix have been taken equal).

The standard deviation S , a measure of broadening of the simulated line profiles, is shown in Fig. 4 as function of the particle/matrix misfit ϵ , for several particle fractions c . The behaviour of $S(\epsilon)$ at small ϵ is influenced by an additional size broadening effect caused by the limited size of the matrix ligament between the non-diffracting particles. This size broaden-

ing effect increases obviously with increasing particle size (see Fig. 4 at $\epsilon = 0$) (and also influences slightly the centroid position (see Fig. 2 at $\epsilon = 0$)). The more or less linear increase in S with ϵ for all c is analogous to the linear relation between line breadth and ϵ as predicted by Eshelby's approach (cf. eqs. (2) and (3) in ref. [5]).

In addition to results for $\langle e_{[11]} \rangle$ and $\sqrt{\langle e_{[11]}^2 \rangle}$, also calculated results for $\langle e_{[10]} \rangle$ and $\sqrt{\langle e_{[10]}^2 \rangle}$ are shown in Fig. 3. Although $\langle e_{[10]} \rangle = \langle e_{[11]} \rangle$, it follows that $\sqrt{\langle e_{[10]}^2 \rangle} \neq \sqrt{\langle e_{[11]}^2 \rangle}$. Hence $\sqrt{\langle e_{[hk]}^2 \rangle}$ is not independent of $[h_m k_m]$. This is in contrast with the results of models based on Eshelby's approach [4–6] and is in particular a consequence of the specific, non-random arrangement of the misfitting particles considered here.

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